

Patent Abstracts of Japan

PUBLICATION NUMBER : 10048157
 PUBLICATION DATE : 20-02-98

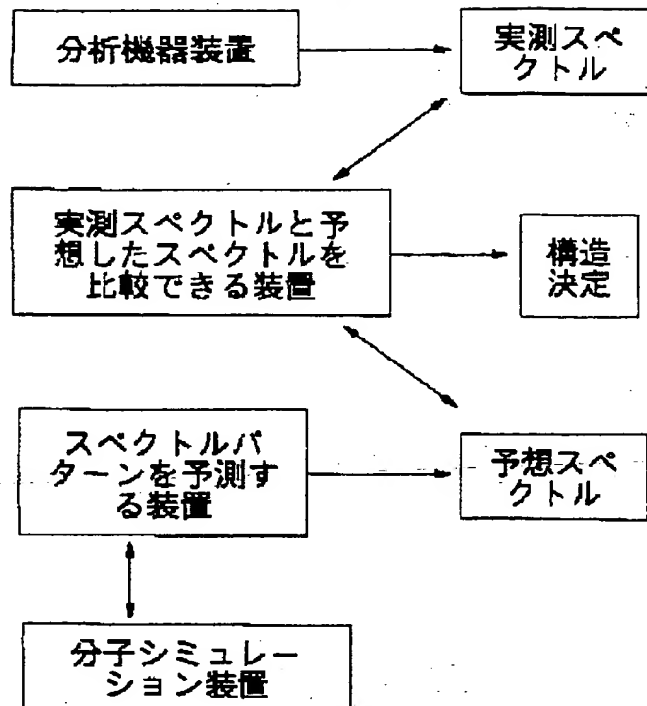
APPLICATION DATE : 08-08-96
 APPLICATION NUMBER : 08209664

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INT.CL. : G01N 23/20 G01N 23/202 // G06F
 17/00

TITLE : APPARATUS FOR MEASURING AND
 ANALYZING WITH SIMULATION OF
 MOLECULE AND METHOD FOR
 ANALYZING CHEMICAL STRUCTURE
 OF SUBSTANCE



ABSTRACT : PROBLEM TO BE SOLVED: To improve the efficiency for analyzing chemical structures of substances and the reliability of results belonging to the structures, by using a device comparing an actual measured spectral pattern of an analyzing device and a spectral pattern estimated by a molecule simulation device, etc.

SOLUTION: An analyzing device is to measure molecular structures and a molecule simulation device is to estimate molecular structures. Moreover, a device for estimating a spectral pattern to be obtained in the analyzing device for a chemical structure estimated in the molecule simulation device, and a device for comparing an actually measured spectral pattern at the analyzing device and the estimated spectral pattern are employed. The analyzing device for measuring the molecular structure reflects the chemical structure of a substance through a spectrum, an image or the like, for example, by X-ray structural diffraction, neutron diffraction, etc. The molecule simulation device is a computer system performing molecular simulation, e.g. by the Monte Carlo calculation method, molecular dynamics calculation method, etc.

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